Amiloride

Model Performance

Model	Data

Weighted KNN model

5-fold CV (75%)		Training (75%)		Test (25%)	
Q2	RMSE	R2	RMSE	R2	RMSE
0.85	0.69	0.86	0.67	0.86	0.78

Model Results

Predicted value: -0.556

Global applicability domain: Inside

Local applicability domain index: 3.76e-01

Confidence level: 6.76e-01

Nearest Neighbors from the Training Set

Image not found
9H-Purine-2,6-diamine, 9-(2-deoxy-beta-D-threo-pentofuranosyl)-
Measured: -0.520
Predicted: -0.625

Image not found
D4DAP
Measured: -0.480
Predicted: -0.407

Image not found
8-Azaguanine
Measured: -0.710
Predicted: -0.407